**RIKILT/WUR BYOD**

Date: 22 November

Address: Akkermaalsbos 2, 6708 WB Wageningen

Province: Gelderland

Phone: 0317 480 256

Directions can be found at:

<https://www.wur.nl/en/Research-Results/Research-Institutes/rikilt.htm>

**Purpose of this document:** This document is an informal document shared by participants of the BYOD meeting. It is open to add information in preparation of the BYOD, and it remains open during the BYOD for notes.

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# **Event information**

Address: Akkermaalsbos 2, 6708 WB Wageningen

Province: Gelderland

Phone: 0317 480 256

Directions can be found at:

<https://www.wur.nl/en/Research-Results/Research-Institutes/rikilt.htm>

Start time: Nov 22: 9:30

End time: Nov 22: 17:30**Goal of the Event**

# 

The goal of the BYOD is to create a FAIR data point for RIKILT’s mycotoxin

data and to demonstrate the benefits of FAIR data to a larger community. The results of this BYOD will be presented on December 12, during the Scientific Symposium on FAIR data science in Wageningen, see: <https://www.wur.nl/en/Value-Creation-Cooperation/WDCC/Show-WDCC/Programme-FAIR-Data-Science.htm>

The BYOD will be split up in two days:

1. One day session to pinpoint/mature research question together with domain experts, find the right ontologies and define semantic data model.
2. Another day session (perhaps online) after a couple of weeks to do the technical work, and to make the FDP operational within Wageningen HPC Infrastructure.

**Driving research questions**

Are we able to combine different data sources within WUR and semantic web resources online based on FAIR data principles.

### **Data Owner Section**

Wheat Mycotoxin Data :

(Cheng)

Crop Passport :

Wheat data from Centre for Genetic Resources (CGN)

Transformation to RDF, ontology “[Multicrop Passport Descriptor](http://www.cropontology.org/ontology/CO_020/FAO-Bioversity%20Multi-Crop%20Passport%20Descriptors)”

(Matthijs / Eliana)

Fusarium :

Fusarium species and their potential toxin profile

Toxin profile was limited to T2-toxin, HT2-toxin, 3ADON, 15-ADON, NIV, Zearalenone and Fumonisin, which are strictly regulated in food and feed. Profile was estimated based on species complex information.

The data was transformed to RDF using a custom perl script.

(Balazs)

# 

# **Interoperability Experts Section**

## **Available** **Linked Data**

*Data that we can easily link to because we have access to it, and experience with.*

* EBI Linked Data sources (<http://www.ebi.ac.uk/rdf/>)
* Agroportal: Crop ontology: <http://www.cropontology.org/>
  + Wheat: <http://www.cropontology.org/ontology/CO_321/Wheat>
* Agrovoc: <http://aims.fao.org/vest-registry/vocabularies/agrovoc>
* CIARD Ring
* Wikidata (general, but has a Tree of Life effort, and collab with GeneWiki)
* Crop Passport : [Centre for Genetic Resources, the Netherlands](https://www.wur.nl/en/Research-Results/Statutory-research-tasks/Centre-for-Genetic-Resources-the-Netherlands-1.html) (Wageningen)
* Ontology of units and measurements: <https://dl.acm.org/citation.cfm?id=2595055> (Wageningen UR)

### Other data sources:

* AgroDataCube: <https://agrodatacube.wur.nl/> (Wageningen UR)
* EPPO Code list: <https://gd.eppo.int/>
* Food Safety Standard EFSA: <https://www.efsa.europa.eu/en/data/data-standardisation>
* GODAN Action Map of Standards in Agriculture and Nutrition: <http://aims.fao.org/vest-registry>
* AgroDataCube: <https://agrodatacube.wur.nl/> (open data from PDOK)
* <https://www.brapi.org/#about>

## **Shared folder for the material created on the BYOD:**

All datasets including raw and metadata in CSV and RDF are available in the GITLab repository of Wageningen University located at git@git.wur.nl:anand.gavai/fairdatapoint\_wur.git

## **Specific Experience of Linked Data experts**

*Please add specific experience*

* Andra Waagmeester - RDF, OWL, SPARQL, Semantic Web Services, SIO ontology
* Rajaram Kaliyaperumal - RDF, SPARQL, Nanopublication, LOVD rdf, Reference Sequence Annotation ontology
* Jan van Lith : Openshift and HPC of Wageningen UR.
* Anand Gavai : Docker, RDF, Semantic Web, Openshift framework of Wageningen UR.
* Cheng Lui : Domain Expert on Wheat, Fusarium and environment.
* Matthijs Brouwer : Domain Expert Crop Passport, RDF, SPARQL
* Evangelia Papoutsoglou : Domain Expert Crop Passport, RDF, SPARQL
* Balazs Brankovics : Domain Expert, Data Steward, RDF, Fungal Data Expert

## **Available infrastructure from within Wageningen University & Research Center.**

1. Gitlab
2. Openshift = Docker + Kubernetes
3. HPC (High Performance Cluster Computation within WUR)
4. GraphDB
5. AllegroGraph

## **Objectives**

Currently RIKILT is sampling Mycotoxin levels in arable crops and they deploy a Mycotoxin prediction model to help farmers to make informed decisions on spraying fungicide. RIKILT would like to improve the prediction models with more data, from available online resources. The data set in concern is a proprietary material from RIKILT on Mycotoxin data from wheat samples collected in the Netherlands. Reason why the Mycotoxin data is interesting and important is because it has several links to multiple domains and is one of international importance to food safety. RIKILT has collected samples from different provinces and recorded agronomy, location specific, environment, cultivar use and analyzed the level of Mycotoxin (a toxic substance for both Human and Animal consumption) in wheat produced by a fungi by the name Fusarium. The objective for this FAIRyfication process is to create a FAIR data point for the RIKILT Mycotoxin sampling data and to reuse existing FAIR data points from other institutions within Netherlands with the hope to improve prediction accuracy of the Mycotoxin prediction models deployed within the WUR .

## **Training Material[[1]](#footnote-0)**

* Linked Data and Ontology Tutorial (powerpoint):<https://onedrive.live.com/view.aspx?resid=40F15725D7B8FBEE!1102&ithint=file%2cpptx&app=PowerPoint&authkey=!AGIKpUwbLzSinIY>
* [Semantic University](http://www.cambridgesemantics.com/nl/semantic-university) provides a series of tutorial material providing a good introduction the semantic web, RDF, SPARQL, etc. It could be worth identifying a subset of these to use as the training material
  + Look at the way that [Software Carpentry](http://software-carpentry.org) is run
* A good book on linked data  
  Tom Heath and Christian Bizer (2011) [*Linked Data: Evolving the Web into a Global Data Space*](http://linkeddatabook.com/editions/1.0/) (1st edition). Synthesis Lectures on the Semantic Web: Theory and Technology, 1:1, 1-136. Morgan & Claypool.
* COEUS documentation: <http://bioinformatics.ua.pt/coeus/documentation/>
* Please post relevant URLs here, including your name and a short description of what can be found there. Examples came from some of the discussions: Andra talked about an open phacts publication oct 2013 about steps towards an rdf. It could be useful to make a list here.
* MOLGENIS documentation <https://github.com/molgenis/molgenis/wiki> and demo <http://molgenis01.target.rug.nl>
* Apache Jena (Java): A free and open source Java framework for building Semantic Web and Linked Data Tutorials: <https://jena.apache.org/tutorials>
* RDF primers : https://www.w3.org/TR/rdf11-concepts/
* RDF vocabulary : <https://www.w3.org/TR/2004/REC-rdf-schema-20040210/>

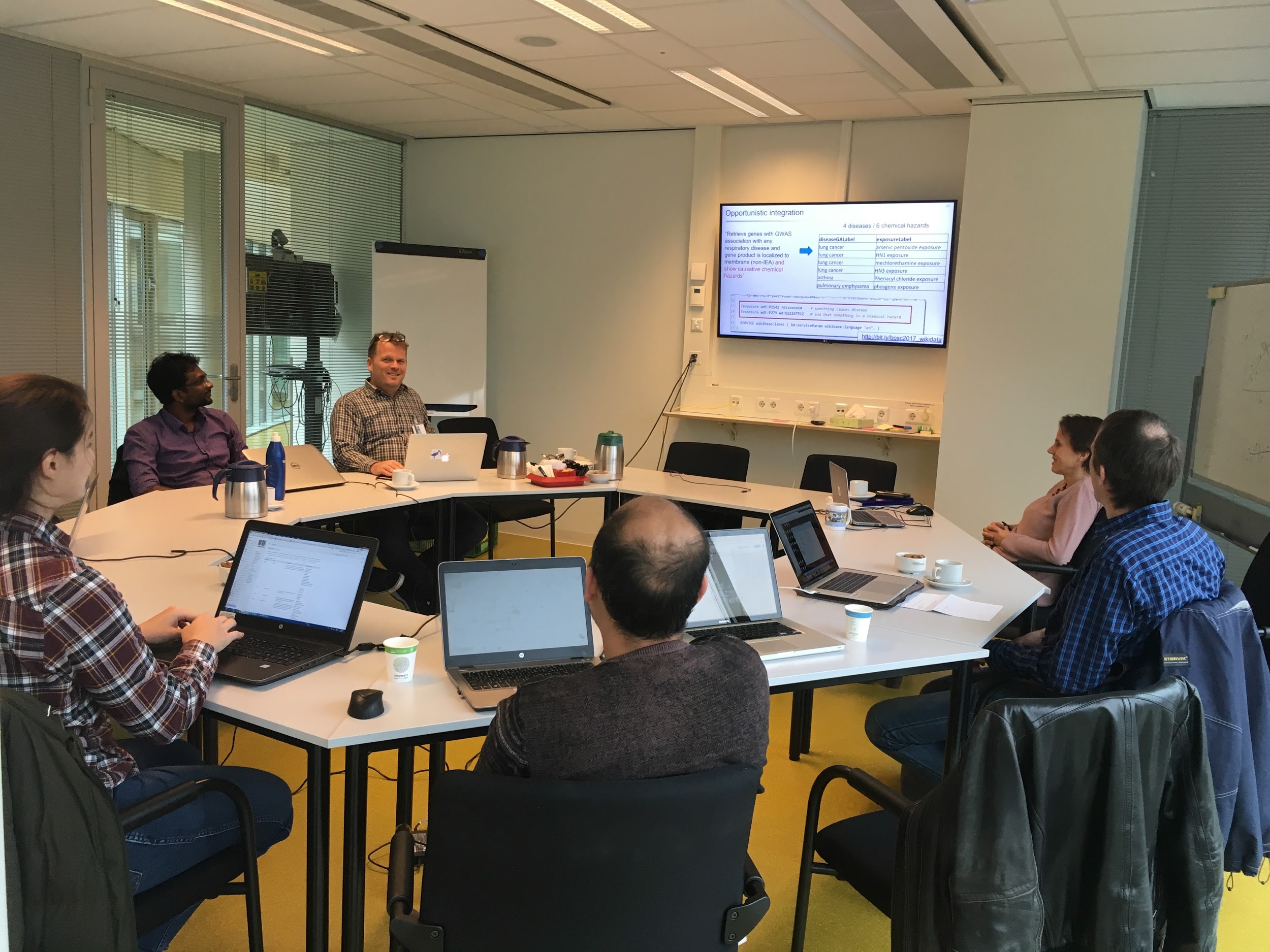
# **Feedback**

## **Day 1**

### **Outcomes**

Outcomes FAIRification of Food Safety Data

In Wageningen we noticed that there is a huge interest in the FAIR data principles and that many are trying to work out how to start making data FAIR. Because we had some earlier experience with Bring Your Own Data (BYOD’s) events we thought it may be nice to pick a Wageningen UR data set to see how far we could get in making the data FAIR and present our findings to the audience of the FAIR data symposium. We anticipated a bumpy road.



At food safety institute RIKILT we found a data set, and above all, a good team to get us started. Naturally, we dreamt of having a perfectly polished FAIR data point that we can use to answer research questions that we could not answer before without being FAIR. However, we knew we had just 2 days to go from nothing to a simple spreadsheet to something that comes a bit closer to FAIR data. The ultimate goal is to reuse existing FAIR data points from other institutions to improve our own research.



The data set from RIKILT is on Mycotoxin data from wheat samples in the Netherlands. Reason why the Mycotoxin data is interesting is because it has several links to multiple domains and is of international importance to food safety. RIKILT collected samples from different provinces and recorded agronomy, basic location, environment, cultivar use and finally analyzed the level of Mycotoxin, a toxic substance in wheat produced by fungi. Currently RIKILT is aiming to improve their Mycotoxin prediction models.

DTL and GO FAIR provided guidance in setting up the FAIRification and contacted external linked data specialists at Micelio. With the help of GODAN expertise on existing standards and ontologies and the domain knowledge of the data owners the linked data experts designed a data model with Micelio started and different domains at Wageningen helped RIKILT to

A BYOD has the following phases:  
\* Extracting a Semantic Data Model

* Here domain experts are key.

\*Finding and identifying the relevant controlled vocabularies and ontologies

* Being part of a community maintaining those ontology is crucial
* Similar to identifying publication venues for scientific literature

\*Generation of FAIR data

\* Create pipelines to transform data to FAIR

\* Requires programming skills

\* Leverage tools like Open Refine

\* Maintain

\* Becoming/Remaining FAIR is a perpetual process.

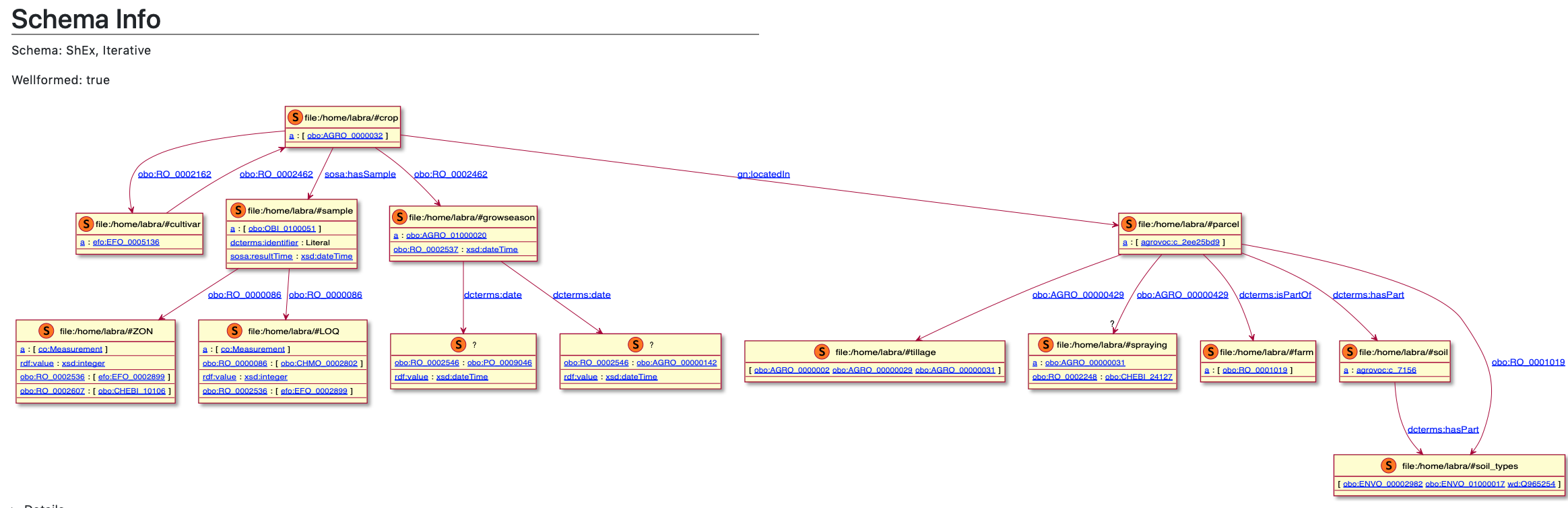
What did we achieve?

**Result 1: A Linked Semantic data model** for the Mycotoxin dataset with references to existing ontologies and vocabularies.

What does this mean?

The concepts or objects in the dataset are more strictly defined and therefore we will be able to compare with other datasets and combine new data more easily. **We learned** that it was very hard to start making a linked data model from scratch.

Our first step was to make sure that everybody gained in depth knowledge about the data set. Naturally we needed the knowledge of the domain experts of RIKILT to achieve that. The next step, was to craft this knowledge in a formal data model, which provides the necessary context to link to other data sets. After all, although laborious and time-consuming, the main idea to go FAIR is to embed this knowledge in a larger context to allow seamless access to heterogeneous knowledge. I.e. being able to for example link plant data with geological, health, statical, food data, etc. This step requires requires shared knowledge descriptions in the form of ontologies and controlled vocabularies. Within the food domain there are already an abundant set of these available, both globally and local. The challenge lies in finding the most suitable controlled vocabularies and ontologies. Finding the right ontologies and controlled vocabularies is a bit similar to finding the right scientific journals to present research outcome, the more experience you have the easier it is to find the right venue and community. Since this exercise is a proof of concept one, he translation of this domain knowledge into a linked data model, proved to be a time consuming challenge, due to the necessity to become knowledgeable of the available ontology space. It would have been ideal if we would have had a good set of ontologies in advance that we could use. We currently have a nice set, but more work is needed to identify and align with other FAIR data communities. B Maturing and alligning ontologies for the food safety community is certainly something to address. etter alignment of the food safety community on a shared data model underpinned by good ontologies and vocabularies would be very useful for successful data science and it would make the FAIRification process much easier. All below deployments are available within the WUR network and can be exposed to the outside world based on GDPR regulations.



**Result 2: A Fair Metadata Editor** is set up to describe the dataset based on the linked data model. In this way the metadata becomes FAIR.

The metadata editor can be found within Wageningen UR hosted HPC cluster at :

<http://fde-rikilt.apps.ocp.wurnet.nl/#!/>

**Result 3: The FAIR Data point** is published on the local infrastructure of Wageningen UR on HPC at:<http://fdp-rikilt.apps.ocp.wurnet.nl/fdp>

**Result 4: The FAIR metadata store (Allegrograph)** is published on the local infrastructure of Wageningen UR HPC at.<http://graph-rikilt.apps.ocp.wurnet.nl/>

**Result 5: The FAIR rdf data store (GraphDB)** is published on the local infrastructure of Wageningen UR HPC at.<http://graphdb-rikilt.apps.ocp.wurnet.nl/>

**Result 6: Identification of related Linked Data communities** Based on a single data set we were able to identify a rich set of relevant ontologies and controlled vocabularies relevant to this domain. Examples: The crop ontology, Agrovoc,

**What did we not achieve?** We could not open the data itself as FAIR data yet, as this would require dealing with privacy and legal aspects as data being sensitive and abiding GDPR regulations !.

**Benefits for RIKILT:**

Making the RIKILT data FAIR has considerable benefits. If the FAIR data principles are followed throughout the institute the data within RIKILT will be FAIR from the beginning. This implies that

by being Findable, Accessible, Interoperable the RIKILT data will become Reusable. Reusable in the classical way of working with data but also machine reusability opens up a whole array of opportunities:

1. to provide better provenance information throughout the institute for more transparency and better accountability.

2. research results from different subdomains can more easily be analyzed.

3. research results from other domains such as environmental data such as weather data or genomic data on fungi or crop cultivars can now be reused more easily. This reuse is throughout the institute and machine readable.

4. Data that is proprietary and cannot be opened to the outside world based on FAIR principles has its own unique selfish motivation of commercial value. Making in house proprietary data FAIR would enable one to combine data from outside to gain more insight into inhouse datasets thus generating new knowledge and opportunity.

5. Models build on FAIR data are self learning as more data becomes available in FAIR format models learn automatically from them and generate new insights.

6. Researchers have the capacity to ask questions that would now cut across scientific domains without having to deal with logistics and bureaucracy.

7. FAIR data principles thus enable and stimulates collaboration based on the reuse of data by making them interoperable for machines.

**Possibilities with FAIR Mycotoxin data**:

**Using environmental data to increase performance of the Mycotoxin prediction model:** With a well defined data model and FAIR metadata it will be easier to link the data set with external data, especially the environmental data of the AgroDataCube would be interesting. According to RIKILT it would be wonderful to see if the additional open data sets on environmental data from the AgroDataCube can increase the performance of the prediction model.

**Automated discovery of new research related to Mycotoxins producing fungi**: Using the FAIR metadata of fungi species (Fusarium) and cultivar (wheat varieties) automatic alerts can be generated for new research findings in journal articles or in FAIR data sets that are published.

**Using Mycotoxin and environmental data for breeding better crop varieties:** Crop passport FAIR data from Wageningen Plant Research can use the Mycotoxin levels produced by certain crop cultivars under certain environmental and management conditions to determine what cultivars are more susceptible to Fusarium and therefore Mycotoxins.

Acknowledgement: I would like to thank all the RIKILT data scientists, and especially Anand Gavai who took up the challenge to identify a data set despite the given time pressure at the end of the year the RIKILT team decided to invest time and effort in this short sprint to make data a bit more FAIR. Also a bit thank you to Mascha Jansen from GO FAIR and Andra Waagmeester and Rajaram Kaliyaperumal who guided us through this journey.



#### Queries example

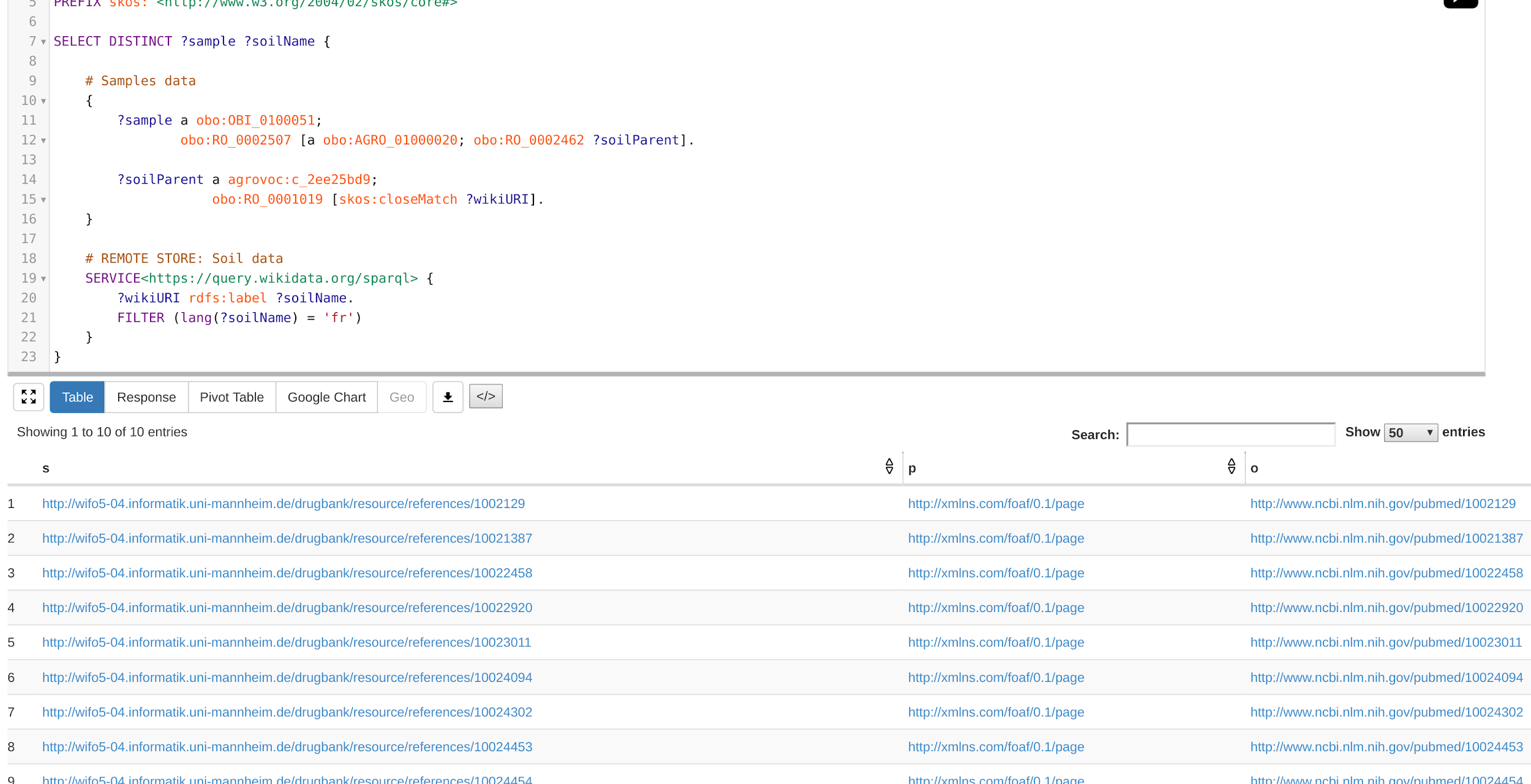
[Source file](https://drive.google.com/open?id=1SN7f398hWcQ7_Blq_EC9ZrrN8GrITSkM)

**1) Get samples and name of the soil in french**

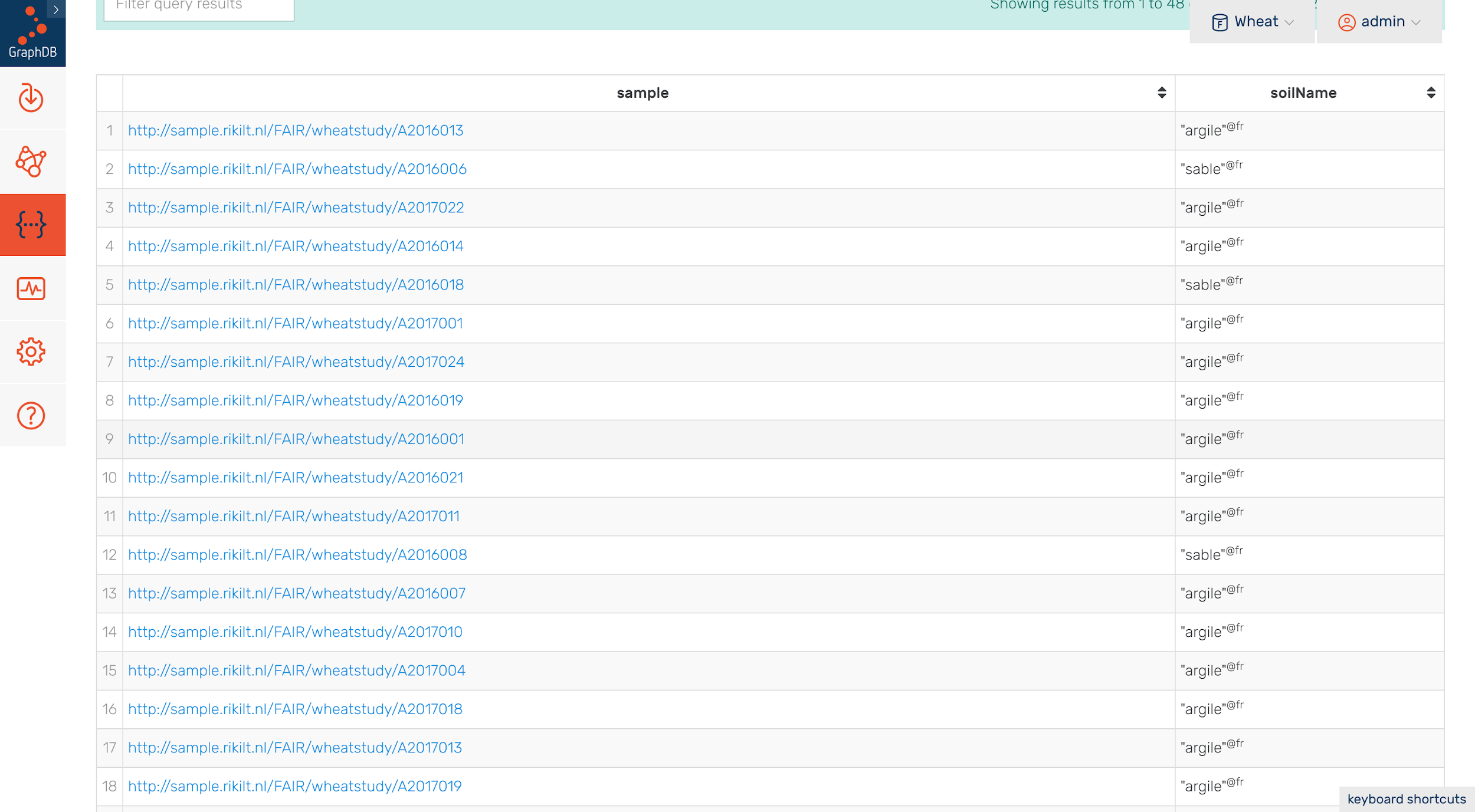
In this query we integrate the wheat dataset with wikidata. we first query wheat data(1) to get samples and soil type and then we query wikidata(2) to get french label of the soil type.

(Join is on Soil type)

**Query**



**Results**

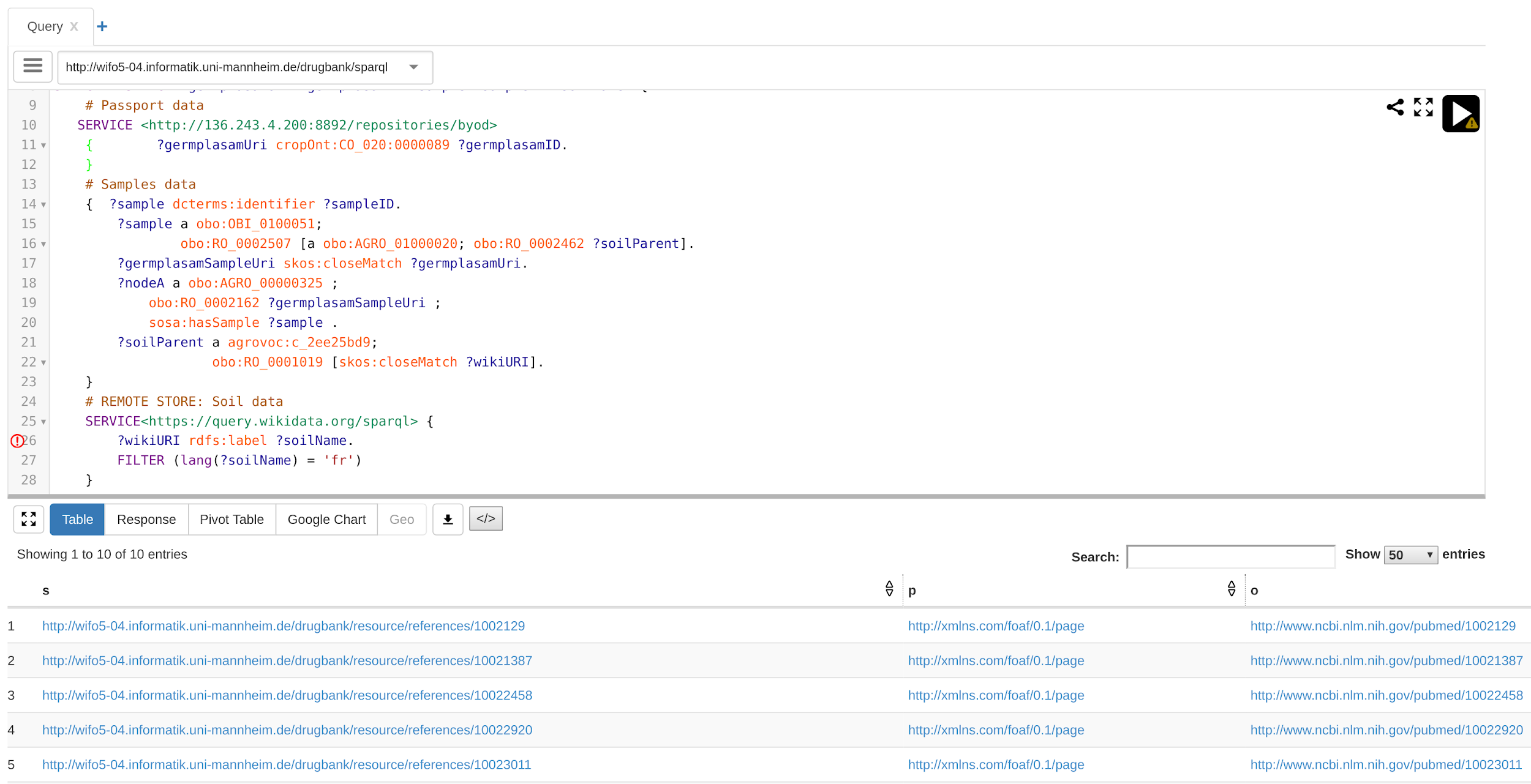
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**2) For a given germplasm ID get samples and name of the soil in french**

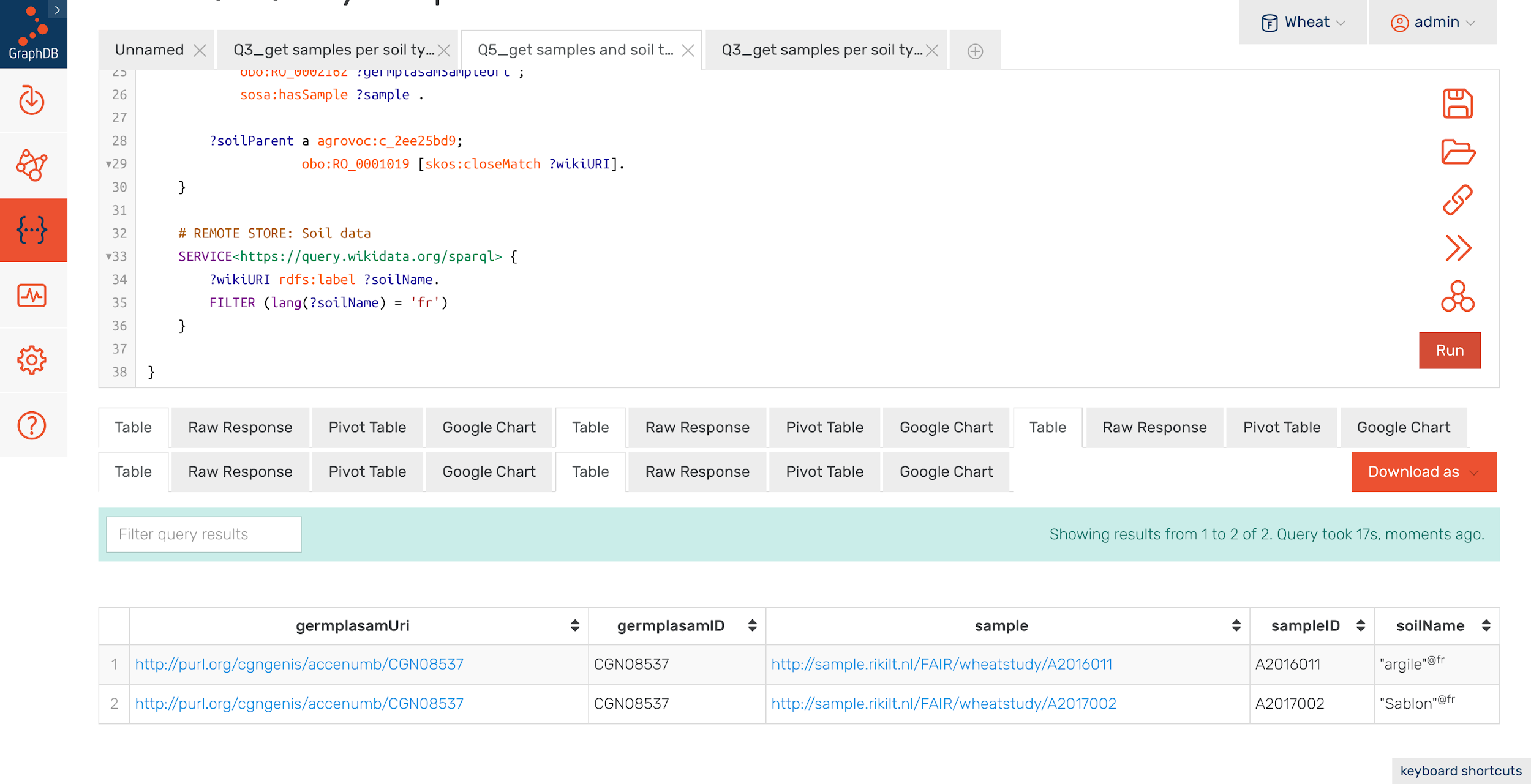
In this query we integrate the crop passport, wheat dataset and wikidata. we first query crop passport data (1) to germplasm URI, for this germplasm uri we query wheat data(2) to get samples and soil type and then we query wikidata(3) to get french label of the soil type.

(Join is on Wheat species & Soil type )

**Query**

****

**Result**

****

### **What went well?**

1. Co-operation between the team members had been excellent.
2. HPC Cluster Support from FB/ICT WUR (Jan Van Lith) had been excellent.

### **Things to take a look at**

Wageningen champions resources:

GODAN related resources:

* VEST Map of standards: https://vest.agrisemantics.org/
* AGROVOC: <http://aims.fao.org/standards/agrovoc/linked-data>
* GACS: <http://agroportal.lirmm.fr/ontologies/GACS>
* Wheat Data Interoperability: <https://www.rd-alliance.org/groups/wheat-data-interoperability-wg.html>
* Cultivar database: <https://gd.eppo.int/>

Wheat data:

* Wheat growth stage ontology: <http://wheat.agroportal.lirmm.fr/ontologies/CO_121>

### **What could have been done? (from data owners perspective)**

### **Preparation for closing session**

# **Parking Lot**

(Points for discussion that come up during the BYOD)

* Youtube using the data train movie: <https://www.youtube.com/watch?v=vUmP8Tli-Mc>

# **BYODers’ Blog**

(Please blog your experience during the BYOD here[[2]](#footnote-1))

Andra: In this stage we are early in developing, to be supportive to the community we should start with use cases where FAIR is used to do things differently from existing methodologies. If the research question can be answered with existing

Ine : Predictive modelling with the aim to forecast.

Ben: would like to showcase tools that are generally applicable within other groups in Wageningen.

Points: Do highlight the limitations of RDF.

How deep are you going to drill down in FAIRification is a critical process,

Ine: Species of grain is important. Harvest happens in September,

Production chain, buyers like to know if it shoul

To Do:

1. Associate ontologies to the semantic model: Andra
   1. Additional data on mycotoxins food safety related: Anand/Cheng
   2. Describe the semantic model in a machine readable schema for validation purposes (Andra)

Eliana: Share the data model she presented.

Plant Phenotype Experiment Ontology (<http://agroportal.lirmm.fr/ontologies/PPEO>)

* + Diagram can be found [here](https://github.com/MIAPPE/MIAPPE/tree/v1.1-rfc/MIAPPE_Checklist-Data-Model-v1.1)

Anand and Cheng: Add information on mycotoxin measurements (1 expand the data model nodes, 2 find ontologies)

Ben to create storylines on why FAIR data is needed: 1 - RIKILT internal data sharing, 2 - RIKILT improving mycotoxin prediction, 3 - Plant Breeding using RIKILT data.

Friday : 07/12/2018

Anand: A quick update from our sprint today.

We started with getting our datasets in order on the git repository at wur. @Rajaram gave us a nice introduction on how to use the fair data editor, fair data point and accordingly @Matthijs and @Balazs and @Cheng created their own metadata available in the git repository including their own datasets were transformed in to RDF.

@Rajaram also showed us the RDF file and the semantic model created by @Andra and it would be good to use these slides during the presentation.

We got stuck with docker-compose on openshift framework @Jan (in CC) did jump in to help us, but we lacked sufficient knowledge on it ! however the FairDataPoint, FairDataEditor and GraphDB are deployed on openshift framework as of now, however they are not able to talk with each other and lack persistent storage. If we are able to establish this on Monday we will be set for the demo on Wednesday!

@Rajaram will check with @Marco if he can make it to Wageningen on Monday, else we will try to sort it out together with Jan and tentatively @Mateusz will join us as we fix it together.

Some noteworthy accomplishments worth mentioning from all the participants today !

Following is the list of datasets that can be found on gitlab of wur at <https://git.wur.nl/anand.gavai/fairdatapoint_wur>:

1. Semantic Data model for wheat Mycotixins (@Andra) this is formalized and available ! not in git yet.

2. RDF of wheat mycotoxin (actual data) (@Andra).

3. Metadata defined for wheat Mycotoxin (@Cheng and @Rajaram).

4. Fusarium RDF and Metadata (@Balazs and @Rajaram)

5. Crop Passport RDF and Metadata (@Matthijs @Rajaram)

6. Data structure organization (@Anand)

7. Docker-compose to Kompose to Openshift (@Anand @Jan and @Mateusz)

8. Data retrieval example (SPARQL) from @Andra combining wheat mycotoxin, soil Ontology and wiki data !

Monday 11/12/2018

Anand: @Anand and @Rajaram started with trying to figure out how the docker compose can be deployed within the openshift HPC cloud of wur. We had to tweak in docker-compose file and @Jan van Lith helped in configuring.

Thus as of today we have 4 pods running as indicated above a Fair Data point (FDP), Fair Data Editor (FDE), Local triple store (Allegro Graph) and a GraphDB (rdf store) all having persistent storage within the HPC cloud of Wageningen UR.

# **APPENDIX**

## **Agenda**

## **November 22, 2018**

### **Morning**

**09:30 - 9:40** Welcome Ben/Karin

**9.40 - 10.00** [Short introduction](https://docs.google.com/presentation/d/1WwUWiwf0azu1kvvqy-Lhz4JZm2qXPUOM5l4YuRaOBtw/edit?usp=sharing) *Andra Waagmeester*

**10:00 - 10:30** Round of introductions by all, what are the expectations and which question and which data sources

**10:30 - 11:00** Coffee break

**11:00 - 12:00** Discussion on research question *Andra Waagmeester & domain experts*Pinpoint research question *Andra Waagmeester & domain experts*

### **Lunch**

### **Afternoon**

**13:00 - 14:00** Workgroup/task/use case division

**14:00 - 15:45** Working session

**15:45 - 16:15** Break

**16:15 - 17:00** Working session 2

**17:00 - 17:30** First impressions / progress report, next steps

**17:30** End of the day

## **Participants List BYOD**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Name** | | **Institute** | **Database/set** | **email** |
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| Balazs Brankovics |  | Biointeractions Group (WUR) |  | balazs.brankovics@wur.nl |
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1. Speical thanks to participants of previous BYODs. [↑](#footnote-ref-0)
2. For reference see Alasdair Gray’s blog of previous BYOD: <http://goo.gl/Hgsyqy> (Alasdair was one of the Linked Data experts) [↑](#footnote-ref-1)